```
=> d hist

     (FILE 'HOME' ENTERED AT 08:54:28 ON 10 FEB 2007)

     FILE 'REGISTRY' ENTERED AT 08:54:45 ON 10 FEB 2007
L1             STRUCTURE UPLOADED
L2              15 S L1 SAM
L3             226 S L1 FULL

     FILE 'CAPLUS, MEDLINE, BIOSIS, EMBASE' ENTERED AT 08:56:52 ON 10 FEB 2007
L4             179 S L3
L5             144 DUPLICATE REMOVE L4 (35 DUPLICATES REMOVED)

     FILE 'REGISTRY' ENTERED AT 08:58:42 ON 10 FEB 2007
L6              29 S L3 AND PROPYL?
L7              29 S L3 AND ?PROPYL

     FILE 'CAPLUS, MEDLINE, BIOSIS, EMBASE' ENTERED AT 09:03:02 ON 10 FEB 2007
L8               1 S 658712-39-1
L9               2 S 328912-19-2

     FILE 'REGISTRY' ENTERED AT 09:05:29 ON 10 FEB 2007
L10             11 S L3 AND PIPERIDIN?

     FILE 'CAPLUS, MEDLINE, BIOSIS, EMBASE' ENTERED AT 09:08:05 ON 10 FEB 2007
L11              2 S 288146-32-7

=>
```

```
NEWS 12   DEC 14  GBFULL and FRFULL enhanced with IPC 8 features and
                  functionality
NEWS 13   DEC 18  CA/CAplus pre-1967 chemical substance index entries enhanced
                  with preparation role
NEWS 14   DEC 18  CA/CAplus patent kind codes updated
NEWS 15   DEC 18  MARPAT to CA/CAplus accession number crossover limit increased
                  to 50,000
NEWS 16   DEC 18  MEDLINE updated in preparation for 2007 reload
NEWS 17   DEC 27  CA/CAplus enhanced with more pre-1907 records
NEWS 18   JAN 08  CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 19   JAN 16  CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 20   JAN 16  IPC version 2007.01 thesaurus available on STN
NEWS 21   JAN 16  WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 22   JAN 22  CA/CAplus updated with revised CAS roles
NEWS 23   JAN 22  CA/CAplus enhanced with patent applications from India
NEWS 24   JAN 29  PHAR reloaded with new search and display fields
NEWS 25   JAN 29  CAS Registry Number crossover limit increased to 300,000 in
                  multiple databases

NEWS EXPRESS  NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
              MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS    STN Operating Hours Plus Help Desk Availability
NEWS LOGIN    Welcome Banner and News Items
NEWS IPC8     For general information regarding STN implementation of IPC 8
NEWS X25      X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that
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* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 08:54:28 ON 10 FEB 2007

=> file reg
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.21       0.21

FILE 'REGISTRY' ENTERED AT 08:54:45 ON 10 FEB 2007
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STRUCTURE FILE UPDATES:    8 FEB 2007  HIGHEST RN 920112-67-0
DICTIONARY FILE UPDATES:   8 FEB 2007  HIGHEST RN 920112-67-0

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.
```
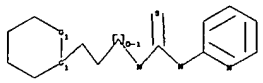
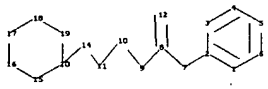

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10726333.str





chain nodes :
7 8 9 10 11 12 14
ring nodes :
1 2 3 4 5 6 15 16 17 18 19 20
chain bonds :
2-7 7-8 8-9 8-12 9-10 10-11 11-14 14-20
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 15-16 15-20 16-17 17-18 18-19 19-20
exact/norm bonds :
2-7 7-8 8-9 8-12 9-10 10-11 11-14 14-20 15-16 15-20 16-17 17-18 18-19 19-20
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

G1:C,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom

L1 STRUCTURE UPLOADED

=> s l1 sam
SAMPLE SEARCH INITIATED 08:55:12 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 42 TO ITERATE

100.0% PROCESSED 42 ITERATIONS 15 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 452 TO 1228
PROJECTED ANSWERS: 68 TO 532

L2 15 SEA SSS SAM L1

```
=> s l1 full
FULL SEARCH INITIATED 08:55:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      918 TO ITERATE

100.0% PROCESSED      918 ITERATIONS                          226 ANSWERS
SEARCH TIME: 00.00.01

L3          226 SEA SSS FUL L1

=> d 1

L3   ANSWER 1 OF 226  REGISTRY  COPYRIGHT 2007 ACS on STN
RN   904127-72-6  REGISTRY
ED   Entered STN:  24 Aug 2006
CN   INDEX NAME NOT YET ASSIGNED
MF   C17 H21 N3 O2 S
SR   Chemical Library
       Supplier: Scientific Exchange, Inc.
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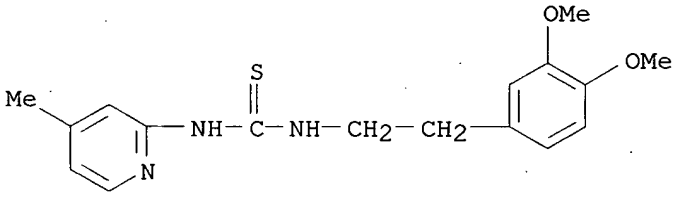


```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**


=> d 226

L3   ANSWER 226 OF 226  REGISTRY  COPYRIGHT 2007 ACS on STN
RN   5454-38-6  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   Thiourea, N-(2-phenylethyl)-N'-2-pyridinyl- (9CI)  (CA INDEX NAME)
OTHER NAMES:
CN   NSC 23099
MF   C14 H15 N3 S
LC   STN Files:   CA, CAPLUS, CASREACT, CHEMCATS, TOXCENTER, USPATFULL
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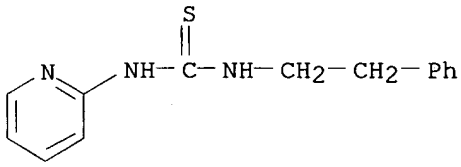


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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

              9 REFERENCES IN FILE CA (1907 TO DATE)
              9 REFERENCES IN FILE CAPLUS (1907 TO DATE)


=> file caplus medline biosis embase
```

```
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                       177.35     177.56

FILE 'CAPLUS' ENTERED AT 08:56:52 ON 10 FEB 2007
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FILE 'BIOSIS' ENTERED AT 08:56:52 ON 10 FEB 2007
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FILE 'EMBASE' ENTERED AT 08:56:52 ON 10 FEB 2007
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=> d hist

     (FILE 'HOME' ENTERED AT 08:54:28 ON 10 FEB 2007)

     FILE 'REGISTRY' ENTERED AT 08:54:45 ON 10 FEB 2007
L1             STRUCTURE UPLOADED
L2              15 S L1 SAM
L3             226 S L1 FULL

     FILE 'CAPLUS, MEDLINE, BIOSIS, EMBASE' ENTERED AT 08:56:52 ON 10 FEB 2007

=> s l3
L4          179 L3

=> duplicate remove l4
DUPLICATE PREFERENCE IS 'CAPLUS, MEDLINE, BIOSIS, EMBASE'
KEEP DUPLICATES FROM MORE THAN ONE FILE?  Y/(N):n
PROCESSING COMPLETED FOR L4
L5           144 DUPLICATE REMOVE L4 (35 DUPLICATES REMOVED)

=> file reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                        16.82     194.38

FILE 'REGISTRY' ENTERED AT 08:58:42 ON 10 FEB 2007
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STRUCTURE FILE UPDATES:     8 FEB 2007  HIGHEST RN 920112-67-0
DICTIONARY FILE UPDATES:    8 FEB 2007  HIGHEST RN 920112-67-0

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  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
```

on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

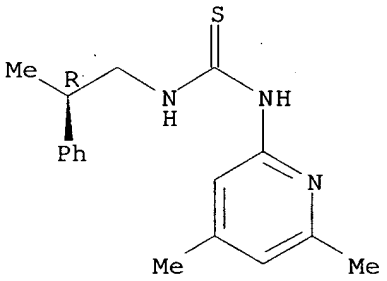
=> 's l3 and propyl?
'S IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> s l3 and propyl?
      2558683 PROPYL?
L6   29 L3 AND PROPYL?

=> d 1-10

L6 ANSWER 1 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 745055-12-3 REGISTRY
ED Entered STN: 15 Sep 2004
CN Thiourea, N-(4,6-dimethyl-2-pyridinyl)-N'-[(2R)-2-phenylpropyl]-
    (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C17 H21 N3 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

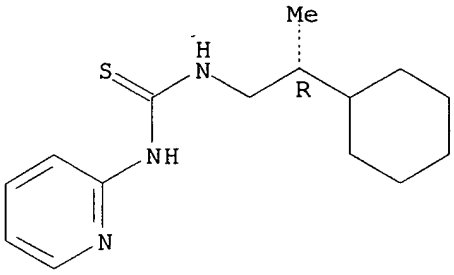


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

            1 REFERENCES IN FILE CA (1907 TO DATE)
            1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 2 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 717908-51-5 REGISTRY
ED Entered STN: 28 Jul 2004
CN Thiourea, N-[(2R)-2-cyclohexylpropyl]-N'-2-pyridinyl- (9CI) (CA
    INDEX NAME)
FS STEREOSEARCH
MF C15 H23 N3 S
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

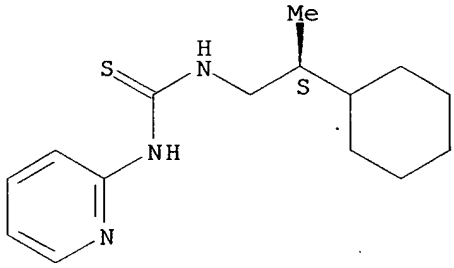


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 3 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 717908-50-4 REGISTRY
ED Entered STN: 28 Jul 2004
CN Thiourea, N-[(2S)-2-cyclohexylpropyl]-N'-2-pyridinyl- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H23 N3 S
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

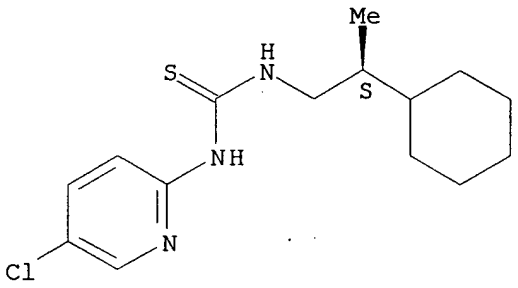


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 4 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 717908-49-1 REGISTRY
ED Entered STN: 28 Jul 2004
CN Thiourea, N-(5-chloro-2-pyridinyl)-N'-[(2S)-2-cyclohexylpropyl]-(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H22 Cl N3 S
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

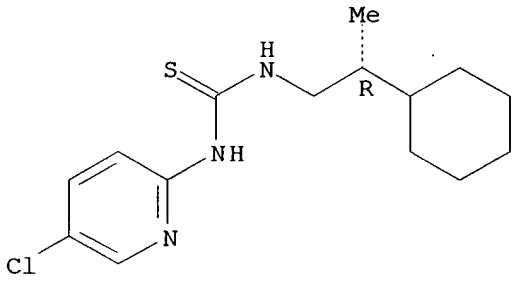


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 5 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 717908-48-0 REGISTRY
ED Entered STN: 28 Jul 2004
CN Thiourea, N-(5-chloro-2-pyridinyl)-N'-[(2R)-2-cyclohexylpropyl]-
(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H22 Cl N3 S
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

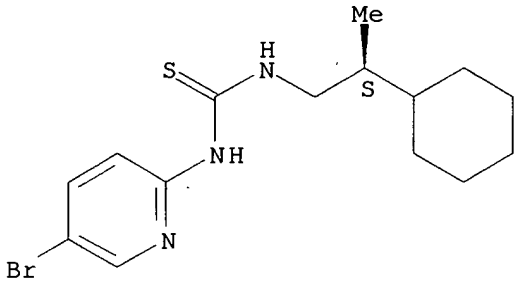


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 6 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 717908-47-9 REGISTRY
ED Entered STN: 28 Jul 2004
CN Thiourea, N-(5-bromo-2-pyridinyl)-N'-[(2S)-2-cyclohexylpropyl]-
(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H22 Br N3 S
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

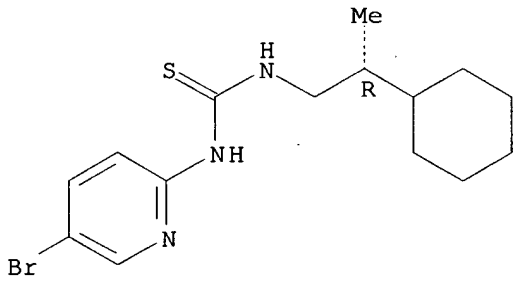


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 7 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 717908-46-8 REGISTRY
ED Entered STN: 28 Jul 2004
CN Thiourea, N-(5-bromo-2-pyridinyl)-N'-[(2R)-2-cyclohexylpropyl]-(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H22 Br N3 S
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

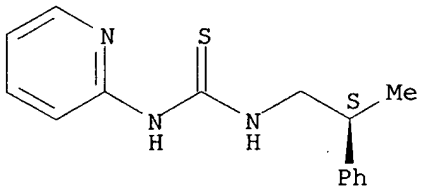


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 8 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 717908-14-0 REGISTRY
ED Entered STN: 28 Jul 2004
CN Thiourea, N-[(2S)-2-phenylpropyl]-N'-2-pyridinyl- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H17 N3 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

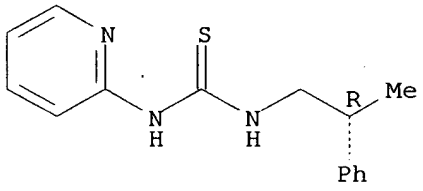


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 9 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 717908-13-9 REGISTRY
ED Entered STN: 28 Jul 2004
CN Thiourea, N-[(2R)-2-phenylpropyl]-N'-2-pyridinyl- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H17 N3 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

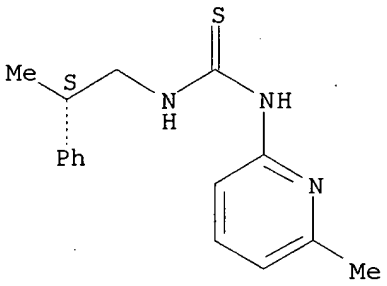


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 10 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 717908-12-8 REGISTRY
ED Entered STN: 28 Jul 2004
CN Thiourea, N-(6-methyl-2-pyridinyl)-N'-[(2S)-2-phenylpropyl]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C16 H19 N3 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.



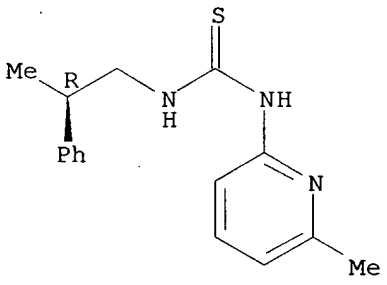
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d 11-29

L6 ANSWER 11 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 717908-11-7 REGISTRY
ED Entered STN: 28 Jul 2004
CN Thiourea, N-(6-methyl-2-pyridinyl)-N'-[(2R)-2-phenylpropyl]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C16 H19 N3 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

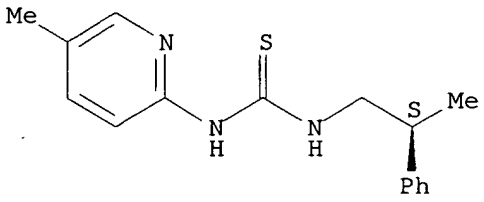


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 12 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 717908-10-6 REGISTRY
ED Entered STN: 28 Jul 2004
CN Thiourea, N-(5-methyl-2-pyridinyl)-N'-[(2S)-2-phenylpropyl]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C16 H19 N3 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

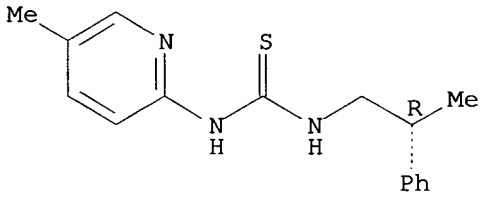


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 13 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 717908-09-3 REGISTRY
ED Entered STN: 28 Jul 2004
CN Thiourea, N-(5-methyl-2-pyridinyl)-N'-[(2R)-2-phenylpropyl]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C16 H19 N3 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

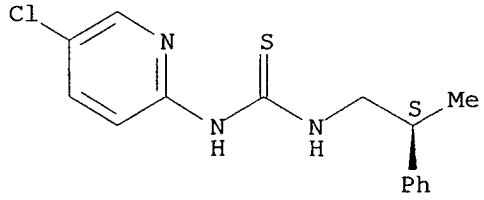


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 14 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 717908-08-2 REGISTRY
ED Entered STN: 28 Jul 2004
CN Thiourea, N-(5-chloro-2-pyridinyl)-N'-[(2S)-2-phenylpropyl]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H16 Cl N3 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

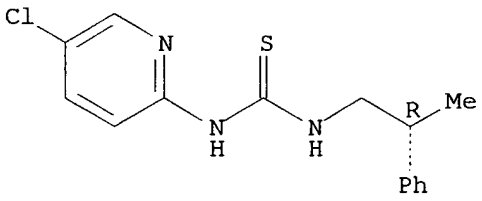


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 15 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 717908-07-1 REGISTRY
ED Entered STN: 28 Jul 2004
CN Thiourea, N-(5-chloro-2-pyridinyl)-N'-[(2R)-2-phenylpropyl]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H16 Cl N3 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

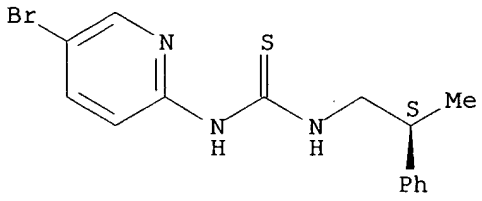


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 16 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 717908-06-0 REGISTRY
ED Entered STN: 28 Jul 2004
CN Thiourea, N-(5-bromo-2-pyridinyl)-N'-[(2S)-2-phenylpropyl]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H16 Br N3 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 17 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 717908-05-9 REGISTRY

ED Entered STN: 28 Jul 2004
CN Thiourea, N-(5-bromo-2-pyridinyl)-N'-[(2R)-2-phenylpropyl]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H16 Br N3 S
SR CA
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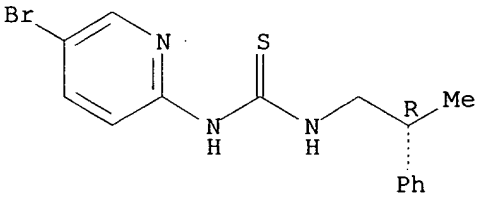
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 18 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 658712-39-1 REGISTRY
ED Entered STN: 05 Mar 2004
CN Thiourea, N-(5-bromo-2-pyridinyl)-N'-[3-(2-methyl-1-piperidinyl)propyl]- (9CI) (CA INDEX NAME)
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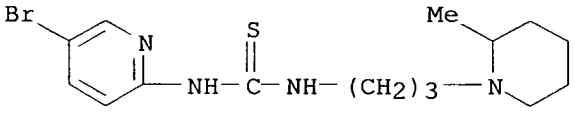
SR CA
LC STN Files: CA, CAPLUS



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1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 19 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 328912-19-2 REGISTRY
ED Entered STN: 26 Mar 2001
CN Thiourea, N-(5-chloro-2-pyridinyl)-N'-[3-(2-methyl-1-piperidinyl)propyl]- (9CI) (CA INDEX NAME)
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SR CA
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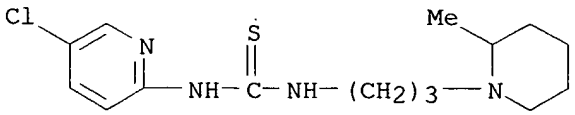

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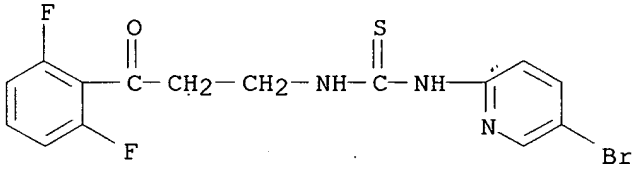
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 20 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 264602-06-4 REGISTRY
ED Entered STN: 12 May 2000
CN Thiourea, N-(5-bromo-2-pyridinyl)-N'-[3-(2,6-difluorophenyl)-3-oxopropyl]- (9CI) (CA INDEX NAME)
MF C15 H12 Br F2 N3 O S
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 21 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 264602-05-3 REGISTRY
ED Entered STN: 12 May 2000
CN Thiourea, N-(5-chloro-2-pyridinyl)-N'-[3-(2,6-difluorophenyl)-3-oxopropyl]- (9CI) (CA INDEX NAME)
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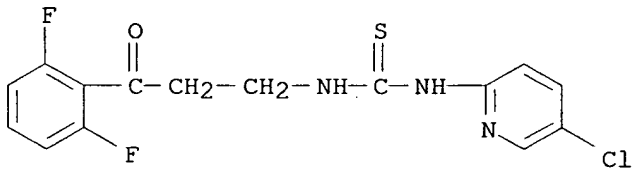
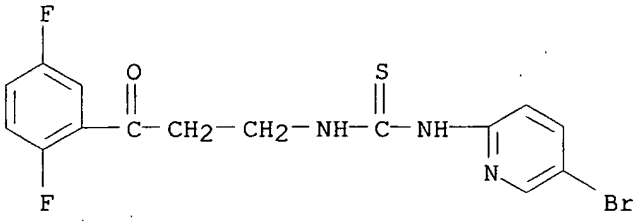
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 22 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 264602-04-2 REGISTRY
ED Entered STN: 12 May 2000
CN Thiourea, N-(5-bromo-2-pyridinyl)-N'-[3-(2,5-difluorophenyl)-3-oxopropyl]- (9CI) (CA INDEX NAME)
MF C15 H12 Br F2 N3 O S
SR CA
LC STN Files: CA, CAPLUS



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1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 23 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 264602-03-1 REGISTRY
ED Entered STN: 12 May 2000
CN Thiourea, N-(5-bromo-2-pyridinyl)-N'-[3-(4-fluorophenyl)-3-oxopropyl]- (9CI) (CA INDEX NAME)
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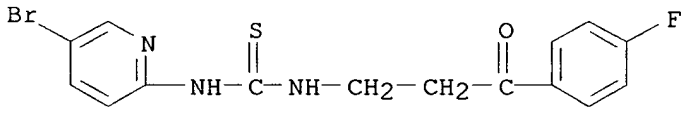
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 24 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 264602-02-0 REGISTRY
ED Entered STN: 12 May 2000
CN Thiourea, N-(5-bromo-2-pyridinyl)-N'-[3-(3-methoxyphenyl)-3-oxopropyl]- (9CI) (CA INDEX NAME)
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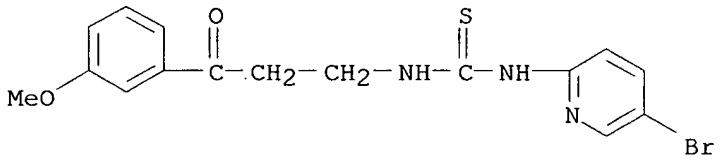
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 25 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 264602-00-8 REGISTRY
ED Entered STN: 12 May 2000
CN Thiourea, N-(5-bromo-2-pyridinyl)-N'-[3-(2-methoxyphenyl)-3-oxopropyl]- (9CI) (CA INDEX NAME)
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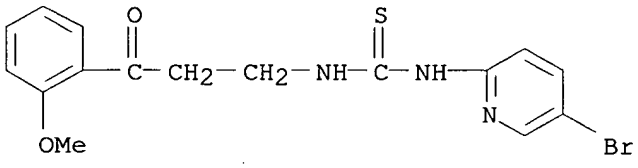
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 26 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 264601-99-2 REGISTRY
ED Entered STN: 12 May 2000
CN Thiourea, N-(5-bromo-2-pyridinyl)-N'-[3-(2-chlorophenyl)-3-oxopropyl]- (9CI) (CA INDEX NAME)
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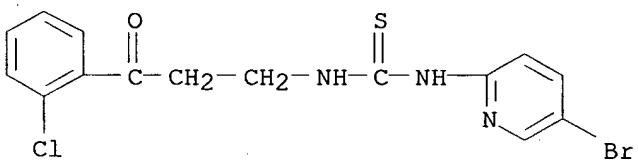
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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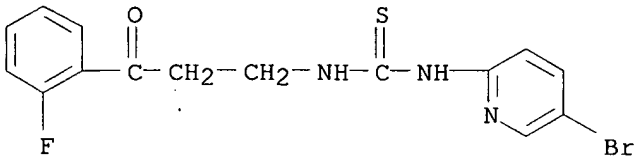
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 27 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 264601-98-1 REGISTRY
ED Entered STN: 12 May 2000
CN Thiourea, N-(5-bromo-2-pyridinyl)-N'-[3-(2-fluorophenyl)-3-oxopropyl]- (9CI) (CA INDEX NAME)
MF C15 H13 Br F N3 O S
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 28 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 264601-97-0 REGISTRY
ED Entered STN: 12 May 2000
CN Thiourea, N-(5-bromo-2-pyridinyl)-N'-(3-oxo-3-phenylpropyl)- (9CI) (CA INDEX NAME)
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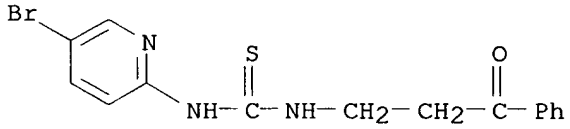
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L6 ANSWER 29 OF 29 REGISTRY COPYRIGHT 2007 ACS on STN
RN 78852-13-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzeneacetamide, 4-chloro-N-[[(5-chloro-2-pyridinyl)amino]thioxomethyl]-α-(1-methylpropyl)- (9CI) (CA INDEX NAME)
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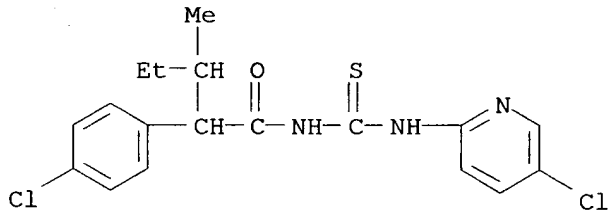
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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     (FILE 'HOME' ENTERED AT 08:54:28 ON 10 FEB 2007)

     FILE 'REGISTRY' ENTERED AT 08:54:45 ON 10 FEB 2007
L1             STRUCTURE UPLOADED
L2           15 S L1 SAM
L3          226 S L1 FULL

     FILE 'CAPLUS, MEDLINE, BIOSIS, EMBASE' ENTERED AT 08:56:52 ON 10 FEB 2007
L4          179 S L3
L5          144 DUPLICATE REMOVE L4 (35 DUPLICATES REMOVED)

     FILE 'REGISTRY' ENTERED AT 08:58:42 ON 10 FEB 2007
L6           29 S L3 AND PROPYL?

=> s l3 and ?propyl
LEFT TRUNCATION IGNORED FOR FILE 'REGISTRY'
       2558683 PROPYL
L7          29 L3 AND ?PROPYL
Left truncation is not valid in the specified search field in the
specified file.  The term has been searched without left truncation.
Examples: '?TERPEN?' would be searched as 'TERPEN?' and '?FLAVONOID'
would be searched as 'FLAVONOID.'

If you are searching in a field that uses implied proximity, and you
used a truncation symbol after a punctuation mark, the system may
interpret the truncation symbol as being at the beginning of a term.
Implied proximity is used in search fields indexed as single words,
for example, the Basic Index.

=> file caplus medline biosis embase
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                     ENTRY    SESSION
FULL ESTIMATED COST                                  69.60     263.98

FILE 'CAPLUS' ENTERED AT 09:03:02 ON 10 FEB 2007
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FILE 'MEDLINE' ENTERED AT 09:03:02 ON 10 FEB 2007

FILE 'BIOSIS' ENTERED AT 09:03:02 ON 10 FEB 2007
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=> s 658712-39-1
L8           1 658712-39-1

=> d ibib abs

L8   ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2003:981015  CAPLUS
DOCUMENT NUMBER:          140:181118
TITLE:                    Structural influence on the anisotropic intermolecular
                          hydrogen bonding in solid state of substituted
                          thioureas: evidence by X-ray crystal structure
AUTHOR(S):                Venkatachalam, T. K.; Sudbeck, E.; Uckun, F. M.
```

CORPORATE SOURCE: Department of Chemistry, Parker Hughes Institute, Roseville, MN, 55113, USA
SOURCE: Journal of Molecular Structure (2004), 687(1-3), 45-56
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The results of an X-ray crystal structure study of 24 substituted thiourea compds. are reported. Comparison of hydrogen bonding characteristics exhibited by structurally distinct thiourea analogs is especially informative concerning the intermol. hydrogen bonding that exists in the crystal structure of individual derivs. In general, all the thiourea derivs. studied showed strong intramol. hydrogen bonding within their structural framework. In addition, among the thioureas studied, with the exception of the 1-(3-aminopropyl)-imidazole substituted thioureas, all other derivs. formed intermol. hydrogen bonding with the thiourea sulfur atom and the NH group. However, we discovered for the first time that the presence of the two nitrogen atoms in the heterocyclic ring of 1-(3-aminopropyl)-imidazolyl substituted thioureas formed the hydrogen bond between the imidazolyl N atom and NH group, consequently eliminating the C:S···NH hydrogen bond formation as shown in the packing of the crystal lattice. The following paper describes this novel anisotropy observed in the intermol. hydrogen bonding among these substituted thiourea derivs. and their salient lattice packing features.

REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

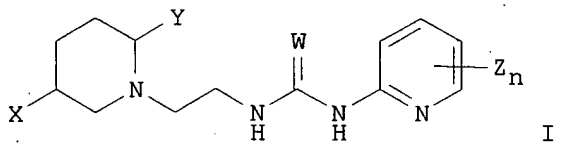
=> s 328912-19-2
L9 2 328912-19-2

=> d ibib abs 1-2

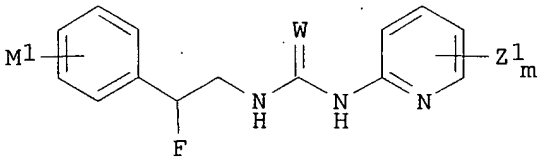
L9 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:794317 CAPLUS
DOCUMENT NUMBER: 137:310817
TITLE: Preparation of piperidinylethyl, phenoxyethyl, and β-fluorophenethyl thioureas with potent anti-HIV activity
INVENTOR(S): Uckun, Fatih M.; Venkatachalam, Taracad K.
PATENT ASSIGNEE(S): Parker Hughes Institute, USA
SOURCE: U.S. Pat. Appl. Publ., 12 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2002151568	A1	20021017	US 2001-6300		20011206
US 6689793	B2	20040210			
PRIORITY APPLN. INFO.:			US 2000-251716P	P	20001206

OTHER SOURCE(S): MARPAT 137:310817
GI



I



II

AB The title compds. [I or II; X, Y, Z, Z1 = H, halo, alkyl, and wherein at least one of X, Y, Z, and Z1 is not H; W = S, O; M1 = Me, Et, halo, etc.; n, m = 1-4] which have been found to be effective non-nucleoside inhibitors (NNRTI) of NNI-resistant and multi-drug resistant human immunodeficiency virus (HIV)-1 reverse transcriptase (RT), were prepared General procedures for synthesis of compds. I or II were described. Biol data for 12 prepared thioureas such as I [W = S; X, Y, Z = H] were given. The present invention is further directed to methods of using the above derivs. I or II to treat patients with NNI-resistant or multi-drug resistant human immunodeficiency virus (HIV)-1.

L9 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:2368 CAPLUS
DOCUMENT NUMBER: 134:202425
TITLE: Piperidinylethyl, phenoxyethyl and fluoroethyl bromopyridyl thiourea compounds with potent anti-HIV activity
AUTHOR(S): Venkatachalam, T. K.; Sudbeck, Elise A.; Mao, Chen; Uckun, Fatih M.
CORPORATE SOURCE: Drug Discovery Program, Department of Chemistry, Parker Hughes Institute, St Paul, MN, 55113, USA
SOURCE: Antiviral Chemistry & Chemotherapy (2000), 11(5), 329-336
CODEN: ACCHEH; ISSN: 0956-3202
PUBLISHER: International Medical Press
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:202425

AB Derivs. of piperidinylethyl, phenoxyethyl and fluoroethyl bromopyridyl thioureas were designed and synthesized as non-nucleoside reverse transcriptase inhibitors (NNRTIs) of HIV-1 reverse transcriptase (RT). The anti-HIV activity of these compds. was examined by determining their ability to inhibit the replication of the HIV-1 strain HTLVIIIB in human peripheral blood mononuclear cells. The unsubstituted parent pyridyl thiourea compound N-[2-(1-piperidine)ethyl]-N'-[2-(pyridyl)]thiourea exhibited no anti-HIV activity, even at 100 μM. However, the thiourea derivs. that contain a bromo- or chloro-substituted pyridyl group, compds. inhibited HIV-1 replication at nanomolar concns. The addition of a Me group onto the piperidine ring significantly altered the potency of these compds.; while Me substitution at the 3-position of the piperidine ring reduced the activity, Me substitution at the 2-position enhanced the anti-HIV activity. The IC50 value of the lead piperidinyl compound, N-[2-(2-methylpiperidinylethyl)]-N'-[2-(5-bromopyridyl)]thiourea was <0.001 μM. All three phenoxyethyl derivs., including the unsubstituted parent phenoxyethyl pyridyl thiourea compound N-[2-(phenoxy)ethyl]-N'-[2-

(pyridyl)]thiourea and the bromo-/chloro-substituted phenoxyethyl halopyridyl thiourea compds. N-[2-(phenoxy)ethyl]-N'-[2-(5-chloropyridyl)]thiourea and N-[2-(phenoxy)ethyl]-N'-[2-(5-bromopyridyl)]thiourea exhibited potent anti-HIV activity with nanomolar IC50 values. The corresponding fluoroethylhalopyridylthiourea compds. β-fluoro[2-phenethyl]-N'[2-(5-chloropyridyl)]thiourea and β-fluoro[2-phenethyl]-N'[2-(5-bromopyridyl)]thiourea inhibited HIV-1 replication in PBMC with subnanomolar IC50 values and selectivity indexes >30000. Compared to the corresponding phenoxyethylthiourea compds., these compds. were >4-5-fold more active as anti-HIV agents. Notably, the lead fluorothiourea compds. were both substantially more active against the NNRTI-resistant HIV strains RTMDR (V106A) and A17 (Y181C) than nevirapine or delavirdine. Taken together, our results provide addnl. exptl. evidence that the structural features of the "linker unit" between the pyridyl and Ph moieties and changes in the Ph group of PETT-related thiourea compds. significantly affects their biol. activity as NNRTIs of HIV-1 RT.

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	16.24	280.22

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.34	-2.34

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 8 FEB 2007 HIGHEST RN 920112-67-0
DICTIONARY FILE UPDATES: 8 FEB 2007 HIGHEST RN 920112-67-0

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> d hist

(FILE 'HOME' ENTERED AT 08:54:28 ON 10 FEB 2007)

FILE 'REGISTRY' ENTERED AT 08:54:45 ON 10 FEB 2007
L1 STRUCTURE UPLOADED
L2 15 S L1 SAM
L3 226 S L1 FULL

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     FILE 'CAPLUS, MEDLINE, BIOSIS, EMBASE' ENTERED AT 08:56:52 ON 10 FEB 2007
L4           179 S L3
L5           144 DUPLICATE REMOVE L4 (35 DUPLICATES REMOVED)

     FILE 'REGISTRY' ENTERED AT 08:58:42 ON 10 FEB 2007
L6            29 S L3 AND PROPYL?
L7            29 S L3 AND ?PROPYL

     FILE 'CAPLUS, MEDLINE, BIOSIS, EMBASE' ENTERED AT 09:03:02 ON 10 FEB 2007
L8             1 S 658712-39-1
L9             2 S 328912-19-2

     FILE 'REGISTRY' ENTERED AT 09:05:29 ON 10 FEB 2007

=> s l3 and piperidin?
       1021724 PIPERIDIN?
L10           11 L3 AND PIPERIDIN?

=> d 1-11

L10  ANSWER 1 OF 11  REGISTRY  COPYRIGHT 2007 ACS on STN
RN   658712-39-1  REGISTRY
ED   Entered STN:  05 Mar 2004
CN   Thiourea, N-(5-bromo-2-pyridinyl)-N'-[3-(2-methyl-1-
     piperidinyl)propyl]- (9CI)  (CA INDEX NAME)
MF   C15 H23 Br N4 S
SR   CA
LC   STN Files:   CA, CAPLUS
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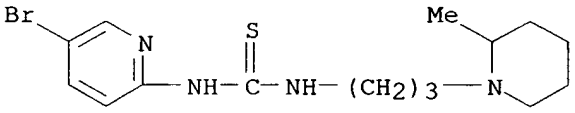


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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

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              1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10  ANSWER 2 OF 11  REGISTRY  COPYRIGHT 2007 ACS on STN
RN   328912-19-2  REGISTRY
ED   Entered STN:  26 Mar 2001
CN   Thiourea, N-(5-chloro-2-pyridinyl)-N'-[3-(2-methyl-1-
     piperidinyl)propyl]- (9CI)  (CA INDEX NAME)
MF   C15 H23 Cl N4 S
SR   CA
LC   STN Files:   CA, CAPLUS, CASREACT, USPAT2, USPATFULL
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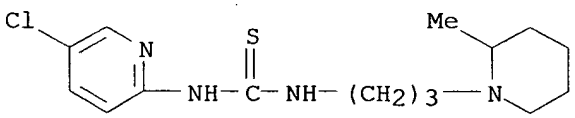


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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

              2 REFERENCES IN FILE CA (1907 TO DATE)
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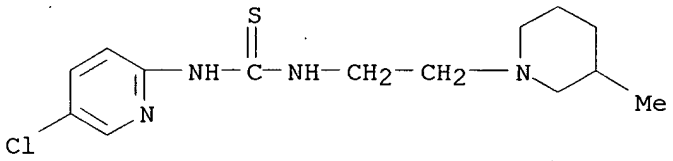
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

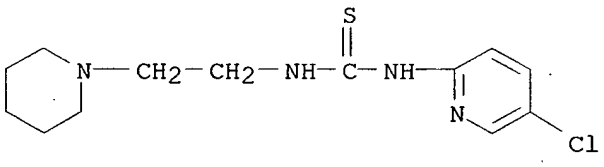
L10 ANSWER 3 OF 11 REGISTRY COPYRIGHT 2007 ACS on STN
RN 328912-17-0 REGISTRY
ED Entered STN: 26 Mar 2001
CN Thiourea, N-(5-chloro-2-pyridinyl)-N'-[2-(3-methyl-1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)
MF C14 H21 Cl N4 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 4 OF 11 REGISTRY COPYRIGHT 2007 ACS on STN
RN 328912-15-8 REGISTRY
ED Entered STN: 26 Mar 2001
CN Thiourea, N-(5-chloro-2-pyridinyl)-N'-[2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)
MF C13 H19 Cl N4 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 5 OF 11 REGISTRY COPYRIGHT 2007 ACS on STN
RN 328912-13-6 REGISTRY
ED Entered STN: 26 Mar 2001
CN Thiourea, N-(5-bromo-2-pyridinyl)-N'-[2-(2-methyl-1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)
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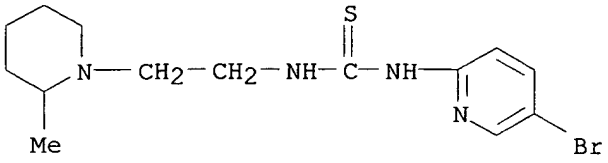
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
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L10 ANSWER 6 OF 11 REGISTRY COPYRIGHT 2007 ACS on STN
RN 328912-11-4 REGISTRY
ED Entered STN: 26 Mar 2001
CN Thiourea, N-(5-bromo-2-pyridinyl)-N'-[2-(3-methyl-1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)
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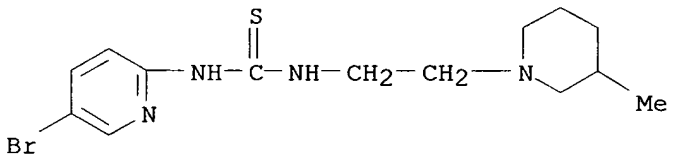
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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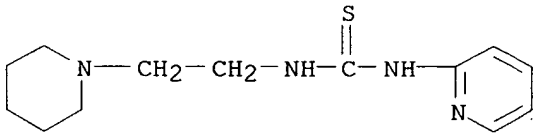
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 7 OF 11 REGISTRY COPYRIGHT 2007 ACS on STN
RN 328912-08-9 REGISTRY
ED Entered STN: 26 Mar 2001
CN Thiourea, N-[2-(1-piperidinyl)ethyl]-N'-2-pyridinyl- (9CI) (CA INDEX NAME)
MF C13 H20 N4 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL

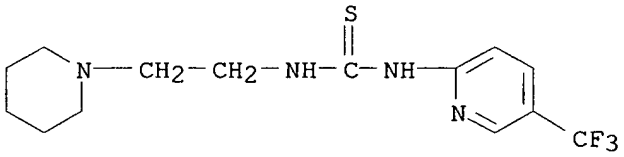


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 8 OF 11 REGISTRY COPYRIGHT 2007 ACS on STN

RN 288146-32-7 REGISTRY
ED Entered STN: 05 Sep 2000
CN Thiourea, N-[2-(1-piperidinyl)ethyl]-N'-[5-(trifluoromethyl)-2-pyridinyl]- (9CI) (CA INDEX NAME)
MF C14 H19 F3 N4 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 9 OF 11 REGISTRY COPYRIGHT 2007 ACS on STN
RN 214753-75-0 REGISTRY
ED Entered STN: 25 Nov 1998
CN Thiourea, N-(5-bromo-2-pyridinyl)-N'-[2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN HI 172
MF C13 H19 Br N4 S
SR CA
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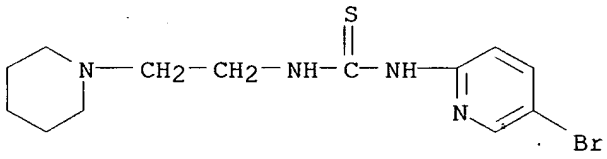
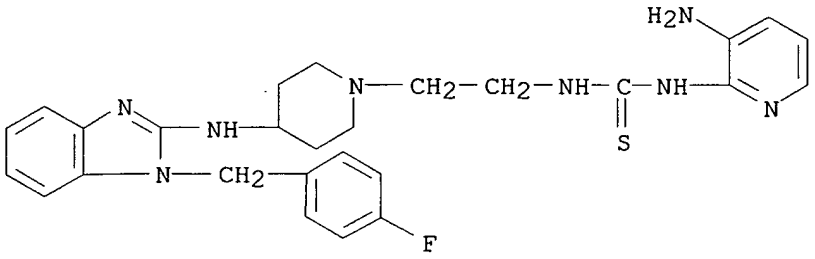


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)
9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

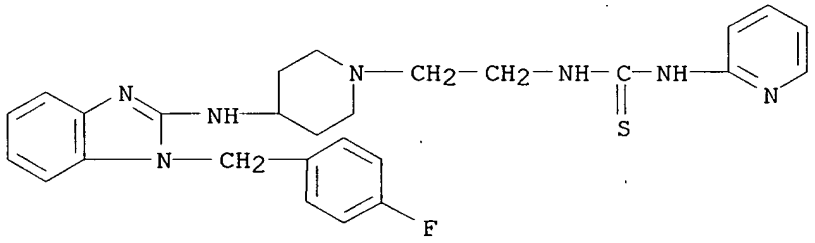
L10 ANSWER 10 OF 11 REGISTRY COPYRIGHT 2007 ACS on STN
RN 90539-27-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN Thiourea, N-(3-amino-2-pyridinyl)-N'-[2-[4-[[1-[(4-fluorophenyl)methyl]-1H-benzimidazol-2-yl]amino]-1-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)
MF C27 H31 F N8 S
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 11 OF 11 REGISTRY COPYRIGHT 2007 ACS on STN
RN 90518-09-5 REGISTRY
ED Entered STN: 16 Nov 1984
CN Thiourea, N-[2-[4-[[1-[(4-fluorophenyl)methyl]-1H-benzimidazol-2-yl]amino]-1-piperidinyl]ethyl]-N'-2-pyridinyl- (9CI) (CA INDEX NAME)
MF C27 H30 F N7 S
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus medline biosis embase

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	28.20	308.42

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.34

FILE 'CAPLUS' ENTERED AT 09:08:05 ON 10 FEB 2007
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FILE 'MEDLINE' ENTERED AT 09:08:05 ON 10 FEB 2007

FILE 'BIOSIS' ENTERED AT 09:08:05 ON 10 FEB 2007

FILE 'EMBASE' ENTERED AT 09:08:05 ON 10 FEB 2007

=> s 288146-32-7
L11 2 288146-32-7

=> d ibib abs 1-2

L11 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:645793 CAPLUS
DOCUMENT NUMBER: 141:168497
TITLE: Dual function thiourea microbicides
INVENTOR(S): Uckun, Fatih M.; D'Cruz, Osmond
PATENT ASSIGNEE(S): Parker Hughes Institute, USA
SOURCE: U.S., 15 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6774139	B1	20040810	US 2000-608710	20000630
US 2004171652	A1	20040902	US 2003-726333	20031201
PRIORITY APPLN. INFO.:			US 2000-608710	B1 20000630

OTHER SOURCE(S): MARPAT 141:168497
AB Contraceptive activity as well as antimicrobial, particularly antiviral protection is provided by contraceptive compns. containing a thiourea compound of the invention exhibiting spermicidal or sperm-immobilizing activity. Preferred compds. of the invention are cyclohexenyl-substituted thiourea compds. For example, thiourea compds. were assayed for their ability to inhibit HIV-1 replication in normal human PBMCs infected with the HIV-1 strain HTLV IIIB as well as for their reverse transcriptase (RT) inhibitory activity in cell-free assays using purified recombinant HIV-1 RT. The sperm immobilizing activity (SIA) of thiourea compds. was evaluated by computer-assisted sperm anal., and the lipophilicity of the compds. was measured by their partition coeffs. between n-octanol and water. The effect of ring substitution and functionalization of the pyridyl moiety of the thiourea derivative, trovirdine was tested.
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:439822 CAPLUS
DOCUMENT NUMBER: 133:159648
TITLE: Novel thiourea compounds as dual-function microbicides
AUTHOR(S): D'Cruz, Osmond J.; Venkatachalam, Taracad K.; Uckun, Fatih M.
CORPORATE SOURCE: Drug Discovery Program, Departments of Reproductive Biology, Parker Hughes Institute, St. Paul, MN, 55113, USA
SOURCE: Biology of Reproduction (2000), 63(1), 196-205
CODEN: BIREBV; ISSN: 0006-3363
PUBLISHER: Society for the Study of Reproduction
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Sexually active women represent the fastest growing human immunodeficiency virus (HIV)/acquired immunodeficiency syndrome risk group. In an effort to develop a vaginal microbicidal contraceptive potentially capable of preventing HIV transmission as well as providing fertility control, we previously reported the synthesis of novel nonnucleoside inhibitors (NNIs)

of HIV-1 reverse transcriptase with sperm-immobilizing activity (SIA). To gain further insight into the structure-function relationship controlling these two properties of NNIs, we have rationally designed and synthesized 30 novel thiourea compds. and examined them for dual-function, anti-HIV and spermicidal activity. Twelve of the 30 thiourea compds. exhibited potent anti-HIV activity in the nanomolar range (IC50 = <1-9 nM). Nine of the 30 thiourea derivs. exhibited both anti-HIV and spermicidal activity. Among the Ph ring-containing thioureas, the 2-fluoro (HI-240) -substituted and 2-chloro (HI-253) -substituted derivs. exhibited potent anti-HIV activity (IC50 = <1 nM) with SIA (EC50 = 70 μM and 147 μM). Among the alicyclic ring-containing thioureas, the 5-bromo (HI-346) and 5-chloro (HI-445) functionalized cyclohexenyl ring-substituted thioureas were the most potent dual-function spermicides (EC50 = 42 and 57 μM), with anti-HIV activity at nanomolar range (IC50 = 3 nM). Unlike nonoxynol-9 (N-9), none of the potent dual-function thiourea compds. were cytotoxic to normal human vaginal, ectocervical, and endocervical epithelial cells at spermicidal concns. We conclude that as potent anti-HIV agents with SIA and reduced cytotoxicity when compared with N-9, the phenyl-substituted and cyclohexenyl-substituted thiourea derivs., especially compds. HI-253 N-[2-(2-chlorophenethyl)]-N'-[2-(5-bromopyridyl)-thiourea], HI-346 N-[2-(5-bromopyridinyl)]-N'-[2-(1-cyclohexenyl)ethyl-thiourea], and HI-445 N-[2-(5-chloropyridinyl)]-N'-[2-(1-cyclohexenyl)ethylthiourea] show unique clin. potential to become the active ingredients of a vaginal contraceptive for women who are at high risk for acquiring HIV by heterosexual vaginal transmission.

REFERENCE COUNT: 70 THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d hist

(FILE 'HOME' ENTERED AT 08:54:28 ON 10 FEB 2007)

FILE 'REGISTRY' ENTERED AT 08:54:45 ON 10 FEB 2007
L1 STRUCTURE UPLOADED
L2 15 S L1 SAM
L3 226 S L1 FULL

FILE 'CAPLUS, MEDLINE, BIOSIS, EMBASE' ENTERED AT 08:56:52 ON 10 FEB 2007
L4 179 S L3
L5 144 DUPLICATE REMOVE L4 (35 DUPLICATES REMOVED)

FILE 'REGISTRY' ENTERED AT 08:58:42 ON 10 FEB 2007
L6 29 S L3 AND PROPYL?
L7 29 S L3 AND ?PROPYL

FILE 'CAPLUS, MEDLINE, BIOSIS, EMBASE' ENTERED AT 09:03:02 ON 10 FEB 2007
L8 1 S 658712-39-1
L9 2 S 328912-19-2

FILE 'REGISTRY' ENTERED AT 09:05:29 ON 10 FEB 2007
L10 11 S L3 AND PIPERIDIN?

FILE 'CAPLUS, MEDLINE, BIOSIS, EMBASE' ENTERED AT 09:08:05 ON 10 FEB 2007
L11 2 S 288146-32-7

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	11.40	319.82

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION

CA SUBSCRIBER PRICE -1.56 -3.90

STN INTERNATIONAL LOGOFF AT 09:11:35 ON 10 FEB 2007

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1617sxw

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS	4	OCT 30	CHEMLIST enhanced with new search and display field
NEWS	5	NOV 03	JAPIO enhanced with IPC 8 features and functionality
NEWS	6	NOV 10	CA/CAplus F-Term thesaurus enhanced
NEWS	7	NOV 10	STN Express with Discover! free maintenance release Version 8.01c now available
NEWS	8	NOV 20	CA/CAplus to MARPAT accession number crossover limit increased to 50,000
NEWS	9	DEC 01	CAS REGISTRY updated with new ambiguity codes
NEWS	10	DEC 11	CAS REGISTRY chemical nomenclature enhanced
NEWS	11	DEC 14	WPIDS/WPINDEX/WPIX manual codes updated
NEWS	12	DEC 14	GBFULL and FRFULL enhanced with IPC 8 features and functionality
NEWS	13	DEC 18	CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS	14	DEC 18	CA/CAplus patent kind codes updated
NEWS	15	DEC 18	MARPAT to CA/CAplus accession number crossover limit increased to 50,000
NEWS	16	DEC 18	MEDLINE updated in preparation for 2007 reload
NEWS	17	DEC 27	CA/CAplus enhanced with more pre-1907 records
NEWS	18	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS	19	JAN 16	CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS	20	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS	21	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS	22	JAN 22	CA/CAplus updated with revised CAS roles
NEWS	23	JAN 22	CA/CAplus enhanced with patent applications from India
NEWS	24	JAN 29	PHAR reloaded with new search and display fields
NEWS	25	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases

NEWS EXPRESS	NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 09:50:45 ON 10 FEB 2007

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 09:50:55 ON 10 FEB 2007
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 8 FEB 2007 HIGHEST RN 920112-67-0
DICTIONARY FILE UPDATES: 8 FEB 2007 HIGHEST RN 920112-67-0

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

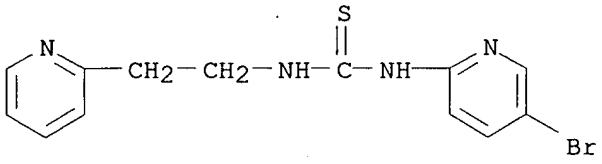
http://www.cas.org/ONLINE/UG/regprops.html

=> s trovirdine
L1 2 TROVIRDINE

=> d 1-2

L1 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2007 ACS on STN
RN 149488-17-5 REGISTRY
ED Entered STN: 20 Aug 1993
CN Thiourea, N-(5-bromo-2-pyridinyl)-N'-[2-(2-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN LY 297345
CN LY 300046
CN PETT
CN Trovirdine
MF C13 H13 Br N4 S
CI COM
SR CA
LC STN Files: ADISINSIGHT, BIOSIS, BIOTECHNO, CA, CAPLUS, CIN, DDFU, DRUGU, EMBASE, IMSDRUGNEWS, IMSRESEARCH, PHAR, PROUSDDR, TOXCENTER, USAN,

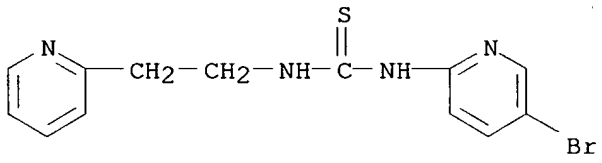
USPAT2, USPATFULL
Other Sources: WHO



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

52 REFERENCES IN FILE CA (1907 TO DATE)
6 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
52 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L1 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2007 ACS on STN
RN 148311-89-1 REGISTRY
ED Entered STN: 25 Jun 1993
CN Thiourea, N-(5-bromo-2-pyridinyl)-N'-[2-(2-pyridinyl)ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)
OTHER NAMES:
CN LY 300046 hydrochloride
CN Trovirdine hydrochloride
MF C13 H13 Br N4 S . Cl H
SR US Adopted Names Council (USAN)
LC STN Files: BIOTECHNO, CA, CAPLUS, EMBASE, IMSRESEARCH, TOXCENTER, USPATFULL
CRN (149488-17-5)



● HCl

5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	11.10	11.31

STN INTERNATIONAL LOGOFF AT 09:54:08 ON 10 FEB 2007